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QUANTUM MECHANICAL DERIVATION OF ENERGY-TEMPERATURE COUPLING.(U)

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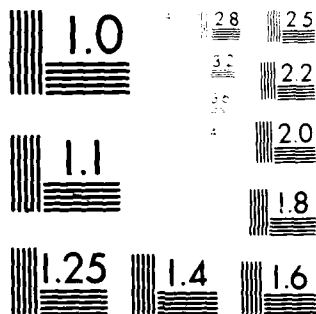
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QUANTUM MECHANICAL DERIVATION OF ENERGY-TEMPERATURE COUPLING

J. Douglas Beason

April 1981

Final Report

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AIR FORCE WEAPONS LABORATORY
Air Force Systems Command
Kirtland Air Force Base, NM, 87117

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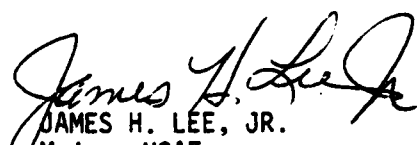
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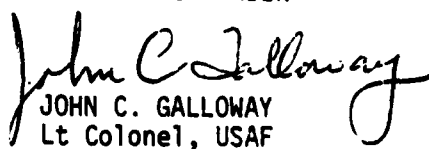
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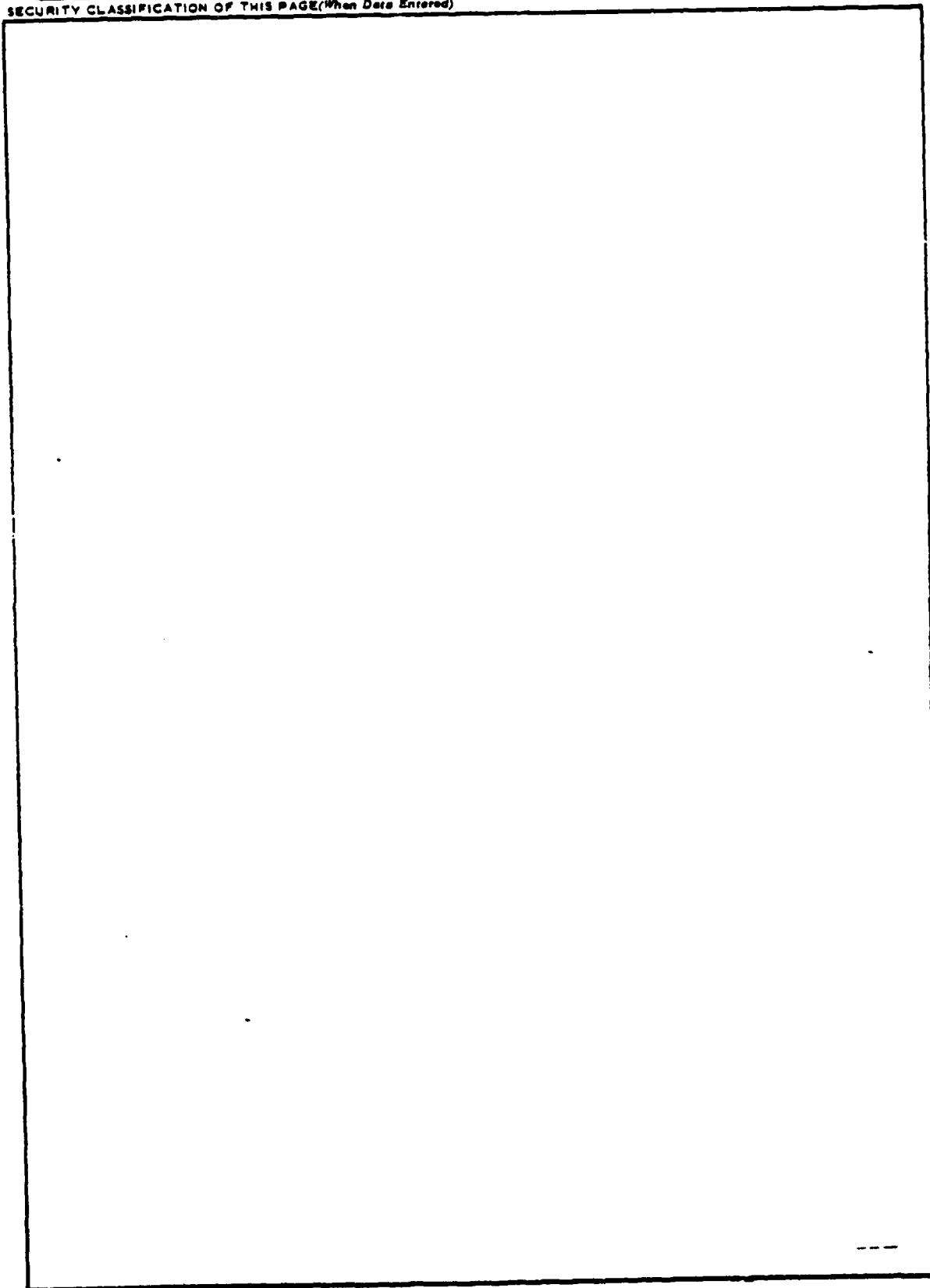
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CONTENTS

<u>Section</u>		<u>Page</u>
I	INTRODUCTION	3
II	THEORY	4
III	CONCLUSIONS	7

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I. INTRODUCTION

Shock wave propagation studies require the use of pressure-energy-volume equations of state (EOS) for the medium through which shocks propagate. It is customary to couple temperature with energy through the use of specific heat and then use temperature with volume to yield pressure. In the case of large gradients of volume and pressure, this technique is invalidated as the coefficients of specific heat depend upon constant (or small changes in) volume and pressure.

Temperature and energy have a more intimate relationship than just specific heat. This report shows the relationship of temperature and energy, so that temperature and energy may still be coupled in the event of large changes in thermodynamic variables. The major part of the following derivation is taken directly from Reference 1.

-
1. Kittel, C., Thermal Physics, John Wiley and Sons, Inc., New York, NY, 1969.

II. THEORY

In a closed quantum mechanical system consisting of N particles, let each particle have two values of "spin": up and down. Spin excess is defined as the difference between the number of particles with spin up and the number of particles with spin down. This is expressed as

$$\text{Spin excess} = (\text{spin up}) - (\text{Spin down}) = 2M \quad (1)$$

If each particle has equal probability of having spin up or spin down, then there are 2^N possible states available for the system to be in.

The generating function for the number of possible states is therefore

$$(X + Y)^N \quad (2)$$

where X = spin up and Y = spin down.

Applying the binomial theorem to Equation 2 yields

$$(X + Y)^N = \sum_{S=0}^N \frac{N!}{(N-S)!S!} X^{N-S} Y^S \quad (3)$$

Note that N is even from Equation 1, if M is an integer. Assuming M to be an integer, M takes all values from $\frac{1}{2}N$ to $-\frac{1}{2}N$. Thus, letting $S = \frac{1}{2}N - M$, Equation 3 is rewritten as

$$(X + Y)^N = \sum_{M=\frac{1}{2}N}^{-\frac{1}{2}N} \frac{N!}{(\frac{1}{2}N + M)!(\frac{1}{2}N - M)!} X^{\frac{1}{2}N+M} Y^{\frac{1}{2}N-M} \quad (4)$$

Note that the coefficient of $X^{\frac{1}{2}N+M} Y^{\frac{1}{2}N-M}$ is the number of states having $\frac{1}{2}N+M$ spins up and $\frac{1}{2}N-M$ spins down [i.e., $(\frac{1}{2}N+M) + (\frac{1}{2}N-M) = N$]. The coefficient of $X^{\frac{1}{2}N+M} Y^{\frac{1}{2}N-M}$ is denoted by $g(N, M)$ where

$$g(N, M) = \frac{N!}{(\frac{1}{2}N + M)!(\frac{1}{2}N - M)!} \quad (5)$$

The $g(N, M)$ is known as the degeneracy function, the number of states having the same value of M .

If two systems are in contact with each other, then the degeneracy of the combined system is simply the product of the degeneracy of the two systems, i.e.,

$$g(N, M) = \sum_{M_1} g_1(N_1, M_1) g_2(N_2, M - M_1) \quad (6)$$

where $M = M_1 + M_2$. Now, if one considers the energy U of a system to be an accessible state of that system, then for the combined system

$$g(N, U) = \sum_{U_1} g_1(N_1, U_1) g_2(N_2, U - U_1) \quad (7)$$

where $U = U_1 + U_2$.

To find the maximum degeneracy g of the combined system, take the first derivative and set it equal to zero, i.e.,

$$d[g(N, U)] = g_2 \left(\frac{\partial g_1}{\partial U_1} \right)_{N_1} dU_1 + g_1 \left(\frac{\partial g_2}{\partial U_2} \right)_{N_2} dU_2 = 0 \quad (8)$$

Dividing each side of Equation 8 by the product $g_1 g_2$ yields

$$\frac{1}{g_1} \left(\frac{\partial g_1}{\partial U_1} \right)_{N_1} = \frac{1}{g_2} \left(\frac{\partial g_2}{\partial U_2} \right)_{N_2} \quad (9)$$

Now recall that

$$\frac{d}{dx} (\log y) = \frac{1}{y} \frac{dy}{dx} \quad (10)$$

Using Equation 9 with the identity of Equation 10 yields

$$\left(\frac{\partial \log g_1}{\partial U_1} \right) = \left(\frac{\partial \log g_2}{\partial U_2} \right) \quad (11)$$

for equilibrium. Note that at this point, the only restriction present in Equation 11 is that the total number of accessible states (N_1 and N_2) remain constant.

In statistical mechanics, entropy is defined as the logarithm of the total number of accessible states in a system. Since the number of accessible states is simply the degeneracy function g , then

$$\sigma(N, U) = \log [g(N, U)] \quad (12)$$

where σ is the entropy. Now, if there are two systems in contact, using Equation 12 with Equation 11 yields

$$\left(\frac{\partial \sigma_1}{\partial U_1} \right)_{N_1} = \left(\frac{\partial \sigma_2}{\partial U_2} \right)_{N_2} \quad (13)$$

in equilibrium.

In statistical mechanics, temperature T is defined

$$\frac{1}{T} = \left(\frac{\partial \sigma}{\partial U} \right)_N \quad (14)$$

This inverse definition of temperature means that energy flows from higher to lower states. It also means that the change in energy of a system is directly related to the temperature as a change in entropy, with only the number of accessible states held constant.

III. CONCLUSIONS

Energy and temperature are directly related by entropy. Pressure and volume do not appear in the definition given in Equation 14. Therefore, if specific heat cannot be used to couple energy and temperature, as in the case of large pressure/volume gradients, then entropy can be used as in Equation 14.